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Ab initio study on spin polarization of III–V compound tips

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Recently, spin electronic states have been found to play an important role under a scanning tunneling microscope (STM) environment [1]. Spin-polarized tunneling has been reported to be observed [2, 3, 4]. Circularly polarized laser beamed on a zinc-blend crystal such as GaAs excites electrons to spin-polarized states. This mechanism has been applied to a Spin-Polarized (SP) STM. Spin-polarized electrons excited in an STM tip tunnel from the tip to the sample surface and are transferred to the unoccupied electronic states of the sample surface with allowed spin states according to the selection rule. Detecting such a tunneling process by STM, we are able to observe surface spin electronic states. On the other hand, in the nanostructure of a surface or in a molecule, spin electronic states may reveal magnetic properties [5, 6, 7]. Extremely high spin states may indicate ferromagnetism [6].

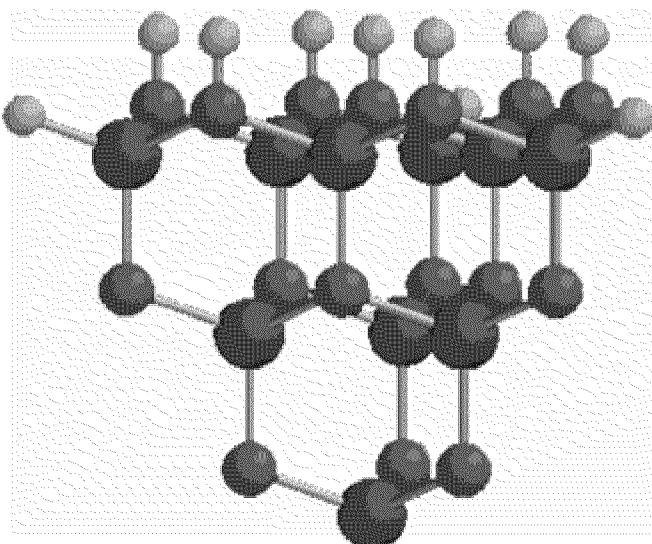


Fig 1. A cluster model for a GaN tip with a Ga atom at the apex in the crystallographic axis (111).

For these systems, the low spin state do not necessarily give the lowest energy. We may be able to design and create nanostructures which have such high spin. In the nanostructure of an STM tip, can electrons be spontaneously spin-polarized due to its geometry? In this study, we will show spin electronics states of GaN tips first and discuss spin polarizability in the nanostructural III–V compound tips. We constructed cluster

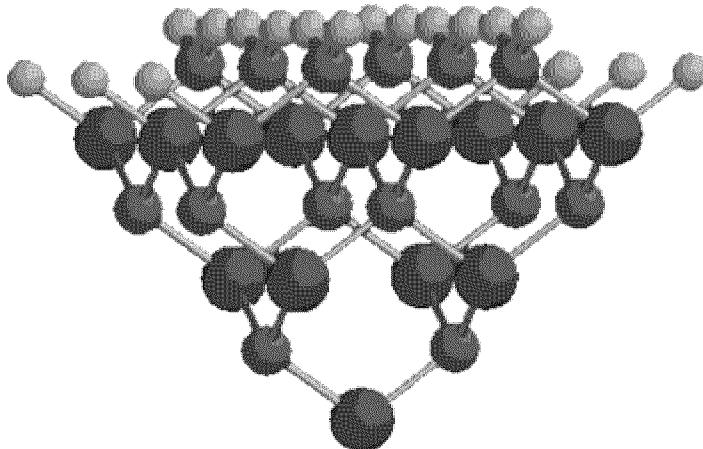


Fig 2. A cluster model for a GaN tip with a Ga atom at the apex in the crystallographic axis (100).

models for STM tips to investigate spin electronic structures of tips comprised of III–V compound materials, using molecular orbital first principles calculations (see Figs. 1 and 2). We used for the models the bulk atomic distances of the corresponding crystalline tips in the zinc-blend structure and terminated the dangling bonds with hydrogen atoms to reproduce the spin electronic states of the crystalline tips. We employed Unrestricted–Hartree–Fock calculations with relativistic effective core potentials. At the apexes of the tips with the axes parallel to the crystallographic axes (111) and (100), electron spins are polarized at the lowest energies. Especially, in case of a GaN tip with a Ga atom at the apex, nearly 10% of the electrons in the valence band are spin-polarized. We performed the above computations for the rest of III–V and some of II–VI compound material tips. It suggests that spin polarizability grows as the difference of electronegativities of the elements of a compound increases and can be enhanced by creating a highly symmetric nanostructure of the tip due to Jahn–Teller effect.

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